

# Quasi Sturmian Basis in Two-Electron Continuum Problems

A. S. Zaytsev<sup>1</sup>, L. U. Ancarani<sup>2</sup>, and S. A. Zaytsev<sup>1</sup>

<sup>1</sup>*Pacific National University, Khabarovsk, 680035, Russia and*

<sup>2</sup>*Equipe TMS, SRSMC, UMR CNRS 7565,*

*Université de Lorraine, 57078 Metz, France*

(Dated: March 13, 2015)

## Abstract

A new type of basis functions is proposed to describe a two-electron continuum which arises as a final state in electron-impact ionization and double photoionization of atomic systems. We name these functions, which are calculated in terms of the recently introduced Quasi Sturmian functions, Convolved Quasi Sturmian functions (CQS). By construction, the CQS functions look asymptotically like a six-dimensional spherical wave. The driven equation describing an  $(e, 3e)$  process on helium in the framework of the Temkin-Poet model has been solved numerically using expansions on the basis CQS functions. The convergence behavior of the solution has been examined as the size of the basis has been increased. The calculations show that the convergence rate is significantly improved by introducing a phase factor corresponding the electron-electron interaction into the basis functions. Such a modification of the boundary conditions leads to appreciable change in the magnitude of the solution.

## I. INTRODUCTION

The Coulomb three-body scattering problem is one of the most fundamental outstanding problems in theoretical atomic and molecular physics. The primary difficulty in description of three charged particles in the continuum is imposing appropriate asymptotic behaviors of the wave function.

Several *ab initio* methods are developed for constructing solutions to the three-body scattering problem (see the review [1]). The exterior complex scaling (ECS) method (see [2] and references therein) allows the problem to be solved without explicit use of the asymptotic boundary conditions. Specifically, ECS recasts the original problem into a boundary problem with zero boundary conditions. (For an extension of ECS to the case of long-range Coulombic interactions see [3, 4].) Some of the other methods use a product of two fixed charge Coulomb waves to approximate the asymptotic three-body continuum state. The convergent close coupling (CCC) [5–7] and the Coulomb-Sturmian separable expansion [8, 9] and the  $J$ -matrix [10, 11] methods treat the problem in the Laguerre basis representation. The latter two methods transform the original problem to a Lippmann-Schwinger-type integral equation whose kernel seems to be generally non-compact. Alternatively, the Generalized Sturmian Functions (GSF) method [12, 13] converts the problem into an inhomogeneous Schrödinger equation with a square integrable driven term. One-particle generalized Sturmian functions with an appropriate asymptotic behavior are obtained (numerically) as eigensolutions of a Sturm-Liouville problem. The GSF method driven equation is solved by an expansion into a basis set of two-particle functions, which are products of two generalized Sturmian functions that both satisfy outgoing-wave boundary conditions [14].

In the present paper in order to describe a Coulomb three-body system continuum we propose a set of two-particle functions, which are calculated by using recently introduced so called Quasi Sturmian (QS) functions [15]. The latter satisfy a two-body inhomogeneous Schrödinger equation with a Coulomb potential and an outgoing-wave boundary condition. Specifically, the two-particle basis functions are obtained, by analogy with the Green's function of two non-interacting hydrogenic atomic systems, as a convolution integral of two one-particle QS functions. The QS functions have the merit that they are expressed in closed form, which allows us to find an appropriate integration path that is useful for numerical calculations of such an integral representation. We name these basis functions Convolved

Quasi Sturmian (CQS) functions. Note that by construction, the CQS function (unlike a simple product of two one-particle ones) looks asymptotically (as the hyperradius  $\rho \rightarrow \infty$ ) like a six-dimensional outgoing spherical wave.

We apply these CQS functions to the solution of a problem of double ionization of He in the framework of the Temkin-Poet model. We solve the driven equation describing an  $(e, 3e)$  process [14] by an expansion into the basis set of CQS functions and explore the convergence properties of the expansion. Note that the CQS functions asymptotic behavior in the so called three-body region  $\Omega_0$  where all three particles are well separated is not correct since it misses out the phase factor, corresponding to the Coulomb interelectronic interaction. Therefore, the expansion method effectiveness is open to question. In order to improve the convergence rate, we equip the basis functions with the phase factor corresponding to the potential  $\frac{1}{r_{12}}$ .

The paper is arranged as follows. In Sec. II we present the three-body driven equations [14] and [16] whose solutions possess all the information for the  $(e, 3e)$  process on helium and that for the one-photon ionization, respectively. Here we suggest the CQS functions which form a basis set used for solving these equations. The CQS functions are expanded in a series of products of the single-particle Laguerre basis functions. A useful integral representation is also introduced for the CQS functions. The asymptotic behavior of the basis functions in the region  $\Omega_0$  is deduced from their integral representation. In this section we also propose a modification of the basis functions which allows to take into account the  $e - e$  interaction. The use of both original and modified versions of the basis functions in solving the  $s$ -wave driven equation [14] is considered in Sec III. Finally, Sec. IV provides a summary. Atomic units are assumed throughout.

## II. QUASI STURMIAN BASIS FUNCTIONS

### A. Driven equations

Electron-impact ionization and double photoionization of atomic systems can be cast as an inhomogeneous three-body Schrödinger equation with a square integrable right hand side. For example, in the approach [14] to the  $(e, 3e)$  process on helium, the four-body Schrödinger equation is reduced to the following driven equation for the three-body system

$(e^-, e^-, \text{He}^{++}) = (1, 2, 3)$ :

$$\left[ E - \hat{H} \right] \Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2) \Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2). \quad (1)$$

$E = \frac{k_1^2}{2} + \frac{k_2^2}{2}$  is the energy of the two ejected electrons. The three-body helium Hamiltonian is given by

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{1}{r_{12}}, \quad (2)$$

$$\hat{H}_j = -\frac{1}{2} \Delta_{r_j} - \frac{2}{r_j}, \quad j = 1, 2. \quad (3)$$

$\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2)$  represents the ground state of the helium atom. The perturbation operator  $\hat{W}_{fi}$  is written as

$$\hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{(2\pi)^3} \frac{4\pi}{q^2} (-2 + e^{i\mathbf{q} \cdot \mathbf{r}_1} + e^{i\mathbf{q} \cdot \mathbf{r}_2}), \quad (4)$$

where  $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$  is the transferred momentum,  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are the momenta of the incident and scattered electrons.

In turn, the one-photon ionization problem also takes the form of the driven equation [16]

$$\left[ E - \hat{H} \right] \Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{2} \vec{\mathcal{E}}_0 \cdot \vec{D}_G \Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2), \quad (5)$$

where  $\vec{\mathcal{E}}_0$  is the amplitude of the electric-field vector and  $\vec{D}_G$  is the dipole operator.

## B. Convolted Quasi Sturmians

Our method of solving the driven equations (1) and (5) is to expand the solution

$$\Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L, \ell, \lambda} \sum_{n_1, n_2=0}^{N-1} C_{n_1 n_2}^{L(\ell_1 \ell_2)} |n_1 \ell_1 n_2 \ell_2; LM\rangle_Q \quad (6)$$

on the basis

$$|n_1 \ell_1 n_2 \ell_2; LM\rangle_Q \equiv \frac{Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2)}{r_1 r_2} \mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \quad (7)$$

$$\mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m_1 m_2=M} (\ell_1 m_1 \ell_2 m_2 | LM) Y_{\ell_1 m_1}(\hat{\mathbf{r}}_1) Y_{\ell_2 m_2}(\hat{\mathbf{r}}_2). \quad (8)$$

Each function  $Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}$  is assumed to satisfy the radial equation

$$\left[ E - \hat{h}_1^{\ell_1} - \hat{h}_2^{\ell_2} \right] Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) = \frac{\psi_{n_1}^{\ell_1}(r_1) \psi_{n_2}^{\ell_2}(r_2)}{r_1 r_2}, \quad (9)$$

where

$$\hat{h}^\ell = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{1}{2}\frac{\ell(\ell+1)}{r^2} - \frac{2}{r}, \quad (10)$$

$\psi_n^\ell$  are the Laguerre basis functions ( $b$  is a real scale parameter)

$$\psi_n^\ell(r) = [(n+1)_{2\ell+1}]^{-\frac{1}{2}} (2br)^{\ell+1} e^{-br} L_n^{2\ell+1}(2br), \quad (11)$$

which are orthogonal with the weight  $\frac{1}{r}$ :

$$\int_0^\infty dr \psi_n^\ell(r) \frac{1}{r} \psi_m^\ell(r) = \delta_{nm}. \quad (12)$$

In order to obtain the  $Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}$  with the outgoing-wave boundary condition we use the Green's function  $\hat{G}^{\ell_1 \ell_2 (+)}(E)$  which can be expressed in the form of the convolution integral [17, 18]

$$\hat{G}^{\ell_1 \ell_2 (+)}(E) = \frac{1}{2\pi i} \int_{\mathcal{C}} d\mathcal{E} \hat{G}^{\ell_1 (+)}(\sqrt{2\mathcal{E}}) \hat{G}^{\ell_2 (+)}(\sqrt{2(E-\mathcal{E})}), \quad (13)$$

where the path of integration  $\mathcal{C}$  in the complex energy plane  $\mathcal{E}$  runs slightly above the branch cut and bound-states poles of  $\hat{G}^{\ell_1 (+)}$  (see Fig. 1). Applying the Green's function operator (which is the inverse of the operator in the left-hand side of (9)) onto both sides of equation (9), we find that

$$Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) = \frac{1}{2\pi i} \int_{\mathcal{C}} d\mathcal{E} Q_{n_1}^{\ell_1 (+)}(\sqrt{2\mathcal{E}}; r_1) Q_{n_2}^{\ell_2 (+)}(\sqrt{2(E-\mathcal{E})}; r_2), \quad (14)$$

where the one-particle quasi Sturmian function  $Q_n^{\ell (+)}$  is defined by [15]

$$Q_n^{\ell (\pm)}(k, r) = \int_0^\infty dr' G^{\ell (\pm)}(k; r, r') \frac{1}{r'} \psi_n^\ell(r'). \quad (15)$$

We name the basis functions (14) Convolutional Quasi Sturmian (CQS).

### C. Laguerre basis expansion

CQS functions can be expanded in terms of the Laguerre basis functions (11) as

$$Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) = \sum_{m_1, m_2=0} \psi_{m_1}^{\ell_1}(r_1) \psi_{m_2}^{\ell_2}(r_2) G_{m_1 m_2, n_1 n_2}^{\ell_1 \ell_2 (+)}(E). \quad (16)$$

The coefficients  $G_{m_1 m_2, n_1 n_2}^{\ell_1 \ell_2 (+)}(E)$  are the matrix elements of the Green's function (13) over the functions

$$\frac{\psi_{n_1}^{\ell_1}(r_1) \psi_{n_2}^{\ell_2}(r_2)}{r_1 r_2} \quad (17)$$

and can be calculated using the convolution [9–11]

$$G_{m_1 m_2, n_1 n_2}^{\ell_1 \ell_2 (+)}(E) = \frac{1}{2\pi i} \int_{\mathcal{C}_1} d\mathcal{E} G_{m_1 n_1}^{\ell_1 (+)}(\sqrt{2\mathcal{E}}) G_{m_2 n_2}^{\ell_2 (+)}(\sqrt{2(E - \mathcal{E})}) \quad (18)$$

of two one-particle Green's function  $G^{\ell (+)}$  matrix elements. The latter is expressed in terms of two independent  $J$ -matrix solutions [19, 20]:

$$G_{mn}^{\ell (+)}(k) = -\frac{2}{k} S_{n < \ell}(k) C_{n > \ell}^{(+)}(k), \quad (19)$$

$$S_{n\ell}(k) = \frac{1}{2} [(n+1)_{(2\ell+1)}]^{1/2} (2 \sin \xi)^{\ell+1} e^{-\pi\beta/2} \omega^{-i\beta} \frac{|\Gamma(\ell+1+i\beta)|}{(2\ell+1)!} \quad (20)$$

$$\times (-\omega)^n {}_2F_1(-n, \ell+1+i\beta; 2\ell+2; 1-\omega^{-2}),$$

$$C_{n\ell}^{(+)}(k) = -\sqrt{n!(n+2\ell+1)} \frac{e^{\pi\beta/2} \omega^{i\beta}}{(2 \sin \xi)^\ell} \times \frac{\Gamma(\ell+1+i\beta)}{|\Gamma(\ell+1+i\beta)|} \frac{(-\omega)^{n+1}}{\Gamma(n+\ell+2+i\beta)} {}_2F_1(-\ell+i\beta, n+1; n+\ell+2+i\beta; \omega^2), \quad (21)$$

where

$$\omega \equiv e^{i\xi} = \frac{b+ik}{b-ik}, \quad \sin \xi = \frac{2bk}{b^2+k^2}, \quad (22)$$

$\beta = \frac{-2}{k}$  is the Sommerfeld parameter. Following the method of [18], we perform the integration in (18) along contour  $\mathcal{C}_1$  (see Fig. 1) which is obtained by rotating the contour  $\mathcal{C}$  by angle  $-\pi < \varphi < 0$  about the point  $\frac{E}{2}$ . This allows us to avoid the singularities of  $G_{m_1 n_1}^{\ell_1 (+)}$ .

Figs. 3 and 4 show the behavior of  $Q_{00}^{00 (+)}$  (16) (the dashed lines) along the  $r_1 = r_2 = \rho/\sqrt{2}$  diagonal. For these calculations, we choose  $E = 0.735$  a.u. and 25 for the upper limit of the sum. The scale parameter  $b$  was set to 1.6875 and the rotation angle  $\varphi$  was  $-\frac{\pi}{3}$ .

#### D. Asymptotic Behavior

The asymptotic form of the QS function  $Q_n^{\ell (\pm)}$  can be written as [15]

$$Q_n^{\ell (\pm)}(k, r) \underset{r \rightarrow \infty}{\sim} -\frac{2}{k} S_{n\ell}(k) e^{\pm i(kr - \beta \ln(2kr) - \frac{\pi\ell}{2} + \sigma_\ell(k))}, \quad (23)$$

where

$$e^{i\sigma_\ell(k)} = \frac{\Gamma(\ell+1+i\beta)}{|\Gamma(\ell+1+i\beta)|}.$$

The asymptotic behavior of the CQS function (14) for  $r_1 \rightarrow \infty$  and  $r_2 \rightarrow \infty$  simultaneously (in the constant ratio  $\tan(\alpha) = r_2/r_1$ , where  $\alpha$  is the hyperangle) is obtained by replacing  $Q_{n_1}^{\ell_1(+)}$  and  $Q_{n_2}^{\ell_2(+)}$  by their asymptotic approximation (23) and making use of the stationary phase method to evaluate the resulting integral. The stationary point  $\mathcal{E}_0$  which satisfies the equation (see, e. g., [21])

$$\frac{\partial}{\partial \mathcal{E}} \left( \sqrt{\mathcal{E}} r_1 + \sqrt{E - \mathcal{E}} r_2 \right) = 0. \quad (24)$$

is  $\mathcal{E}_0 = \cos^2(\alpha)E$ . Therefore, we finally obtain

$$Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) \underset{\rho \rightarrow \infty}{\sim} \frac{1}{E} \sqrt{\frac{2}{\pi}} (2E)^{3/4} e^{\frac{i\pi}{4}} S_{n_1 \ell_1}(p_1) S_{n_2 \ell_2}(p_2) \frac{1}{\sqrt{\rho}} \\ \times \exp \left\{ i \left[ \sqrt{2E} \rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2) + \sigma_{\ell_1}(p_1) + \sigma_{\ell_2}(p_2) - \frac{\pi(\ell_1 + \ell_2)}{2} \right] \right\}, \quad (25)$$

where  $\rho = \sqrt{r_1^2 + r_2^2}$  is the hyper-radius,  $p_1 = \cos(\alpha)\sqrt{2E}$ ,  $p_2 = \sin(\alpha)\sqrt{2E}$ ,  $\beta_{1,2} = \frac{-2}{p_{1,2}}$ .

### E. Integral representation

Rather than apply the expansion (16) to calculate the CQS functions at large distances, it might be more convenient to employ the contour integral (14) whose integrand is expressed in terms of the integral [15]

$$Q_n^{\ell(\pm)}(k, r) = -[(n+1)_{2\ell+1}]^{-\frac{1}{2}} (2br)^{\ell+1} e^{-br} \frac{2}{(b \mp ik)} \int_0^1 dz (1-z)^{\ell \pm i\alpha} (1 - \omega^{\pm 1} z)^{\ell \mp i\alpha} \\ \times (1 - z - \omega^{\pm 1} z)^n \exp(z[b \pm ik]r) L_n^{2\ell+1} \left( \frac{(1-z)(1-\omega^{\pm 1} z)}{(1-z-\omega^{\pm 1} z)} 2br \right). \quad (26)$$

Note that a part of the rotated straight-line contour  $\mathcal{C}_1$  indicated by a dashed line in Fig. 1 lies in the unphysical energy sheet ( $-2\pi < \arg(\mathcal{E}) < 0$ ). In turn,  $Q_n^{\ell(+)}(\sqrt{2\mathcal{E}}, r)$  diverges exponentially for large  $\text{Im}(\mathcal{E})$  (see, e.g., (23)) in the lower half-plane. In order to ensure convergence of the integral (14) we deform the contour  $\mathcal{C}_1$  in such a way that the resulting path  $\mathcal{C}_2$ , shown in Fig. 2, asymptotically approaches the real axis. Specifically, the energy  $\mathcal{E}$  on the contour  $\mathcal{C}_2$  is parametrized in the form

$$\mathcal{E} = t + iD \frac{(\frac{E}{2} - t)}{1 + t^2}, \quad (27)$$

where  $D$  is a positive constant and  $t$  runs from  $\infty$  to  $-\infty$ . Generally there are points on the contour  $\mathcal{C}_2$  at which  $\text{Re}(\ell + i\beta) < -1$  and thus the integrand in (26) is singular at the endpoint  $z = 1$ . To avoid this, we apply the following procedure. Let  $m$  be the minimum

positive integer number such that  $-m < \text{Re}(\ell + i\beta)$ . Then integrating (26) by part  $m - 1$  times and assuming the integrated terms vanish at the limit  $z = 1$  we obtain the integral which can be evaluated numerically. As a test of this analytic continuation of  $Q_n^{\ell(+)}(k, r)$  into the complex  $k$ -plane, the CQS function  $Q_{00}^{00(+)}$  has been calculated using the integral (14) along the contour  $\mathcal{C}_2$ . We choose  $D = 0.85$  for which  $m = 3$ . The results for real and imaginary parts are plotted in Fig. 3 and Fig. 4 by the solid lines. We also plot the CQS function  $Q_{00}^{00(+)}$  calculated with  $D = 15$  for which  $-1 < \text{Re}(i\beta)$ , i.e.,  $m = 1$  (the dashed lines). Agreement between these representations of CQS functions and (16) argues for the suggested analytic continuation.

Note that the asymptotic behavior (25) of the two-particle CQS functions depends upon the indices  $n_1$  and  $n_2$ . It follows from (20) that this dependence can be eliminated by dividing (14) by  $B_{n_1}^{\ell_1}(p_1)B_{n_2}^{\ell_2}(p_2)$ , where

$$B_n^\ell(k) = [(n+1)_{2\ell+1}]^{1/2} (-\omega)^n {}_2F_1(-n, \ell+1+i\beta; 2\ell+2; 1-\omega^{-2}). \quad (28)$$

We present in Figs. 5 and 6 a few  $s$ -wave CQS functions  $Q_{n_1 n_2}^{00(+)}/B_{n_1}^0(p_1)B_{n_2}^0(p_2)$  for  $\alpha = \frac{\pi}{4}$ . These functions asymptotic behavior at large distances is shown in Figs. 7 and 8. For comparison, we also show the asymptotic approximation (25) for  $Q_{00}^{00(+)}$ .

Note that it follows from (26) that on the left part of the contour  $\mathcal{C}_2$  where  $k \sim i|k|$  and  $|k| \rightarrow \infty$  the function  $Q_n^{\ell(+)}$  for large  $r$  behaves like  $e^{-br}$  rather than  $e^{ikr}$ . Thus, the greater is the scale parameter  $b$ , the faster the CQS function (14) reaches its asymptotic form (25).

## F. The solution asymptotic form

We try to solve the equation (1) by an expansion into the basis set of CQS functions (7) whose asymptotic behavior in the region  $\Omega_0$  is not correct since it misses out at least the phase factor, corresponding to the Coulomb interelectronic interaction (see, e. g., [21, 22]):

$$W_3(\mathbf{r}_1, \mathbf{r}_2) = -\frac{\rho}{\sqrt{2E}} \frac{1}{r_{12}} \ln \left( 2\sqrt{2E}\rho \right). \quad (29)$$



Inserting (25) into (6) we find the formal result for the asymptotic form of the solution of (1) at large distances:

$$\begin{aligned} \Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) &\approx \frac{2}{E \sin(2\phi)} \sqrt{\frac{2}{\pi}} (2E)^{3/4} e^{\frac{i\pi}{4}} \frac{\exp\{i[\sqrt{2E}\rho - \alpha_1 \ln(2p_1 r_1) - \alpha_2 \ln(2p_2 r_2)]\}}{\rho^{5/2}} \\ &\times \sum_{\ell_1 \ell_2 L} \mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \exp\left\{i\left[\sigma_{\ell_1}(p_1) + \sigma_{\ell_2}(p_2) - \frac{\pi(\ell_1 + \ell_2)}{2}\right]\right\} \\ &\times \sum_{n_1, n_2=0}^{N-1} C_{n_1 n_2}^{L(\ell_1 \ell_2)} S_{n_1 \ell_1}(p_1) S_{n_2 \ell_2}(p_2). \end{aligned} \quad (30)$$

Thus the feasibility of using the CQS functions (7) for solving (1) is questionable. To improve the asymptotic properties of the CQS function (and thereby solve the problem of slow convergence of the expansion (6)), it may be useful to modify the CQS function by multiplying it by

$$e^{i\mathcal{W}_{\ell_1 \ell_2}(r_1, r_2)}, \quad (31)$$

where

$$\mathcal{W}_{\ell_1 \ell_2}(r_1, r_2) \underset{\rho \rightarrow \infty}{\sim} -\frac{\rho}{\sqrt{2E}} \mathcal{V}_{\ell_1 \ell_2}(r_1, r_2) \ln(2\sqrt{2E}\rho), \quad (32)$$

$$\mathcal{V}_{\ell_1 \ell_2}(r_1, r_2) = \int d\hat{\mathbf{r}}_1 d\hat{\mathbf{r}}_2 [\mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)]^* \frac{1}{r_{12}} \mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \quad (33)$$

Hence the modified function takes the form

$$\tilde{Q}_{n_1, n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2) = e^{i\mathcal{W}_{\ell_1 \ell_2}(r_1, r_2)} Q_{n_1, n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2). \quad (34)$$

Note, however, that such phase factors can not take into account the off-diagonal elements

$$\mathcal{V}_{\ell_1 \ell_2, \ell'_1 \ell'_2}(r_1, r_2) = \int d\hat{\mathbf{r}}_1 d\hat{\mathbf{r}}_2 [\mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)]^* \frac{1}{r_{12}} \mathcal{Y}_{LM}^{\ell'_1 \ell'_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \quad (35)$$

Thus, it will probably be more convenient to choose the basis functions of the form

$$e^{iW_3(\mathbf{r}_1, \mathbf{r}_2)} |n_1 \ell_1 n_2 \ell_2; LM\rangle_Q. \quad (36)$$

It is beyond the scope of this paper to discuss in detail the modified basis functions and their applications. In this report we restrict ourselves to a simple  $s$ -wave case.

### III. SOLVING OF THE DRIVEN EQUATION

In the Temkin-Poet model the equation (1) reduces to [14]

$$\left[ E + \frac{1}{2} \frac{\partial^2}{\partial r_1^2} + \frac{1}{2} \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{r_{>}} \right] \chi(r_1, r_2) = \mathcal{F}(r_1, r_2), \quad (37)$$

where  $\chi(r_1, r_2) = r_1 r_2 \phi^{(+)}(r_1, r_2)$ , whereas the right hand side is given by

$$\mathcal{F}(r_1, r_2) = -\frac{1}{(2\pi)^3} \frac{4\pi}{q^2} [2 - j_0(qr_1) - j_0(qr_2)] r_1 r_2 \frac{Z_e^3}{\pi} e^{-Z_e(r_1+r_2)}. \quad (38)$$

We set  $E = 0.735$ ,  $q = 0.24$  and  $Z_e = 2 - 5/16$ .

To solve the equation we first consider the expansion

$$\chi(r_1, r_2) = \sum_{n_1, n_2=0}^{N-1} C_{n_1, n_2} Q_{n_1, n_2}^{(+)}(r_1, r_2). \quad (39)$$

Our discussion is limited to  $s$  waves, so that we omit the angular-momentum labels  $\ell_1$  and  $\ell_2$ . We choose  $Z_e$  for the scale parameter  $b$  of the basis. Inserting (39) into (37) gives

$$\sum_{n_1, n_2=0}^{N-1} \left[ \frac{\psi_{n_1}(r_1) \psi_{n_2}(r_2)}{r_1 r_2} - \frac{1}{r_>} Q_{n_1, n_2}^{(+)}(r_1, r_2) \right] C_{n_1, n_2} = \mathcal{F}(r_1, r_2). \quad (40)$$

Then, multiplying Eq. (40) by  $\psi_{m_1}(r_1) \psi_{m_2}(r_2)$  and integrating, in view of the orthogonality condition (12), gives

$$\sum_{n_1, n_2=0}^{N-1} [\delta_{m_1, n_1} \delta_{m_2, n_2} + \mathcal{L}_{m_1, m_2; n_1, n_2}] C_{n_1, n_2} = \mathcal{R}_{m_1, m_2}, \quad m_1, m_2 \leq N-1, \quad (41)$$

where

$$\mathcal{R}_{m_1, m_2} = \int_0^\infty \int_0^\infty dr_1 dr_2 \psi_{m_1}(r_1) \psi_{m_2}(r_2) \mathcal{F}(r_1, r_2). \quad (42)$$

Further, we approximate the matrix elements

$$\mathcal{L}_{m_1, m_2; n_1, n_2} \equiv \int_0^\infty \int_0^\infty dr_1 dr_2 \psi_{m_1}(r_1) \psi_{m_2}(r_2) \left( -\frac{1}{r_>} \right) Q_{n_1, n_2}^{(+)}(r_1, r_2) \quad (43)$$

by using the expansion of CQS function into the Laguerre basis (16) and taking into account the basis completeness:

$$\mathcal{L}_{m_1, m_2; n_1, n_2} = - \sum_{n'_1, n'_2=0}^{N-1} V_{m_1, m_2; n'_1, n'_2} G_{n'_1, n'_2; n_1, n_2}^{(+)}, \quad (44)$$

where  $V_{m_1, m_2; n'_1, n'_2}$  are the matrix elements of the  $e - e$  interaction:

$$V_{m_1, m_2; n'_1, n'_2} = \int_0^\infty \int_0^\infty dr_1 dr_2 \psi_{m_1}(r_1) \psi_{m_2}(r_2) \frac{1}{r_>} \psi_{n'_1}(r_1) \psi_{n'_2}(r_2). \quad (45)$$

Our aim is to study the convergence properties of the expansion (39) (in conjunction with the approximation (44)) as  $N$  is increased. The real and imaginary parts of the solution  $\chi(r_1, r_2)\rho^{1/2}2/\sin 2\alpha = \phi^{(+)}\rho^{5/2}$  along the  $r_1 = r_2 = \rho/\sqrt{2}$  diagonal are shown in Figs. 9 and 10. Figures 11 and 12 show the results for the asymptotic approximation (30) (multiplied by  $\rho^{5/2}$ ) to the solution. From the plots we see that applying the expansion (39) yields a solution with divergent phase as a function of  $N$ , whereas the magnitude

$$A \equiv \lim_{\rho \rightarrow \infty} |\phi^{(+)}(r_1, r_2)\rho^{5/2}| \quad (46)$$

seems to converge. Actually, from the asymptotic form (30) of the solution, it follows that

$$A_N = \frac{2(2E)^{3/4}}{E \sin 2\alpha} \sqrt{\frac{2}{\pi}} \frac{1}{4\pi} \left| \sum_{n_1, n_2=0}^{N-1} C_{n_1, n_2} S_{n_1}(p_1) S_{n_2}(p_2) \right|. \quad (47)$$

In the case  $\alpha = \frac{\pi}{4}$ ,  $p_1 = p_2 = \sqrt{E}$  we have obtained  $A_{16} = 1.505 \times 10^{-4}$ ,  $A_{21} = 1.507 \times 10^{-4}$  and  $A_{26} = 1.400 \times 10^{-4}$ .

It might be expected that the convergence could be achieved using the modified CQS functions:

$$\tilde{Q}_{n_1, n_2}^{(+)}(r_1, r_2) \equiv e^{i\mathcal{W}(r_1, r_2)} Q_{n_1, n_2}^{(+)}(r_1, r_2), \quad (48)$$

$$\mathcal{W}(r_1, r_2) = -\frac{\rho}{\sqrt{2E}} \frac{1}{(1 + r_>)} \ln \left( 2\sqrt{2E}(1 + \rho) \right). \quad (49)$$

Then substituting the expansion

$$\tilde{\chi}(r_1, r_2) = \sum_{n_1, n_2=0}^{N-1} \tilde{C}_{n_1, n_2} \tilde{Q}_{n_1, n_2}^{(+)}(r_1, r_2). \quad (50)$$

into (37) gives

$$\sum_{n_1, n_2=0}^{N-1} \left[ \frac{\psi_{n_1}(r_1)\psi_{n_2}(r_2)}{r_1 r_2} - \hat{U} Q_{n_1, n_2}^{(+)}(E; r_1, r_2) \right] \tilde{C}_{n_1, n_2} = e^{-i\mathcal{W}(r_1, r_2)} \mathcal{F}(r_1, r_2), \quad (51)$$

where the operator  $\hat{U}$  is defined by

$$\begin{aligned} \hat{U} = & \frac{1}{r_>} + \frac{1}{2} \left( \frac{\partial \mathcal{W}}{\partial r_1} \right)^2 + \frac{1}{2} \left( \frac{\partial \mathcal{W}}{\partial r_2} \right)^2 - \frac{i}{2} \left( \frac{\partial^2 \mathcal{W}}{\partial r_1^2} + \frac{\partial^2 \mathcal{W}}{\partial r_2^2} \right) \\ & - i \left[ \frac{\partial \mathcal{W}}{\partial r_1} \frac{\partial}{\partial r_1} + \frac{\partial \mathcal{W}}{\partial r_2} \frac{\partial}{\partial r_2} \right]. \end{aligned} \quad (52)$$

For large  $\rho$  one finds from (25) that

$$\frac{\partial}{\partial r_{1,2}} Q_{n_1, n_2}^{(+)}(E; r_1, r_2) \sim i\sqrt{2E} \frac{r_{1,2}}{\rho} Q_{n_1, n_2}^{(+)}(E; r_1, r_2), \quad (53)$$

and therefore the action of  $\hat{U}$  on  $Q_{n_1, n_2}^{(+)}$  in the asymptotic region is reduced to multiplication by the ‘effective potential’

$$U_{n_1, n_2}^{eff}(r_1, r_2) \equiv \frac{\hat{U}Q_{n_1, n_2}^{(+)}(E; r_1, r_2)}{Q_{n_1, n_2}^{(+)}(E; r_1, r_2)}, \quad (54)$$

such that

$$U_{n_1, n_2}^{eff}(r_1, r_2) \underset{\rho \rightarrow \infty}{\sim} \left( \frac{\ln(2\sqrt{2E}\rho)}{\sqrt{2E}\rho} \right)^2. \quad (55)$$

Figure 13 shows plots of the  $U_{00}^{eff}$  and  $U_{55}^{eff}$  on the diagonal  $r_1 = r_2$ . For comparison we have also plotted the  $e - e$  potential  $\frac{1}{r_{>}}$ .

A matrix equation for the coefficients  $\tilde{C}_{n_1, n_2}$  is obtained by multiplying (51) from the left by  $\psi_{m_1}(r_1)\psi_{m_2}(r_2)$  and integrating over both coordinates:

$$\sum_{n_1, n_2=0}^{N-1} \left[ \delta_{m_1, n_1} \delta_{m_2, n_2} + \tilde{\mathcal{L}}_{m_1, m_2; n_1, n_2} \right] \tilde{C}_{n_1, n_2} = \tilde{\mathcal{R}}_{m_1, m_2}, \quad m_1, m_2 \leq N-1, \quad (56)$$

where

$$\tilde{\mathcal{R}}_{m_1, m_2} = \int_0^\infty \int_0^\infty dr_1 dr_2 \psi_{m_1}(r_1) \psi_{m_2}(r_2) e^{-i\mathcal{W}(r_1, r_2)} \mathcal{F}(r_1, r_2), \quad (57)$$

$$\tilde{\mathcal{L}}_{m_1, m_2; n_1, n_2} = - \sum_{n'_1, n'_2=0}^{N-1} U_{m_1, m_2; n'_1, n'_2} G_{n'_1, n'_2; n_1, n_2}^{(+)}, \quad (58)$$

$$U_{m_1, m_2; n'_1, n'_2} = \int_0^\infty \int_0^\infty dr_1 dr_2 \psi_{m_1}(r_1) \psi_{m_2}(r_2) \hat{U} \psi_{n'_1}(r_1) \psi_{n'_2}(r_2). \quad (59)$$

Figures 14 and 15 show the solution  $\tilde{\chi}(r_1, r_2) \rho^{1/2} 2 / \sin 2\alpha = \tilde{\phi}^{(+)} \rho^{5/2}$  along the diagonal  $r_1 = r_2$ . In turn, figures 16 and 17 present the real and imaginary components of the corresponding asymptotic form

$$\begin{aligned} \tilde{\phi}^{(+)} \rho^{5/2} \underset{\rho \rightarrow \infty}{\sim} & \frac{2(2E)^{3/4}}{E \sin 2\alpha} \sqrt{\frac{2}{\pi}} \frac{1}{4\pi} \sum_{n_1, n_2=0}^{N-1} \tilde{C}_{n_1, n_2} S_{n_1}(p_1) S_{n_2}(p_2) \exp \left( -i \frac{\rho}{\sqrt{2E}} \frac{1}{r_{>}} \ln(2\sqrt{2E}\rho) \right) \\ & \times \exp \left\{ i \left[ \sqrt{2E}\rho - \alpha_1 \ln(2p_1 r_1) - \alpha_2 \ln(2p_2 r_2) + \sigma_0(p_1) + \sigma_0(p_2) + \frac{\pi}{4} \right] \right\}. \end{aligned} \quad (60)$$

From the plots one can see that the convergence can be achieved by introducing a phase factor corresponding to the interelectronic potential  $1/r_{12}$ . Furthermore, such a modification of the asymptotic form of the basis functions could result in appreciable change in the solution magnitude

$$\tilde{A} \equiv \lim_{\rho \rightarrow \infty} \left| \tilde{\phi}^{(+)}(r_1, r_2) \rho^{5/2} \right|. \quad (61)$$

For comparison, in this case we have obtained  $\tilde{A}_{16} = 7.346 \times 10^{-4}$ ,  $\tilde{A}_{21} = 7.396 \times 10^{-4}$  and  $\tilde{A}_{26} = 7.593 \times 10^{-4}$ .

#### IV. SUMMERY

Two-particle basis functions — labelled CQS — are proposed. By analogy with the Green's function of two non-interacting hydrogenic atomic systems, they are expressed as a convolution integral of two one-particle QS functions. We suggest an analytic continuation of the QS functions into the entire complex  $k$ -plane in order to perform the numerical contour integration. The asymptotic limit of the CQS basis functions in the region  $\Omega_0$  is expressed in closed form as a six-dimensional outgoing spherical wave.

We study the application of the expansion into the CQS functions to the solution of the inhomogeneous equation describing the double ionization of helium by high-energy electron impact in the framework of the Temkin-Poet model. Note that in constructing the basis functions we do not take into account the interelectronic interaction, and therefore the asymptotic behavior of the basis functions is not correct. Hence, the driven equation whose solution is expanded in terms of these basis functions is noncompact (due to the Coulomb potential  $\frac{1}{r_{12}}$  in the left hand side). Thus the applicability of this approach is questionable. We show that the problem of slow convergence (or even perhaps lack of convergence) of the expansion can be solved by using the modified CQS functions equipped with the phase factor corresponding to the potential  $\frac{1}{r_{12}}$ . Moreover, the solutions which satisfy the different boundary conditions differ appreciably in magnitude. These results suggest that suitable basis functions can be obtained by expanding products of the missing phase factor and CQS functions in series of bispherical harmonics.

#### Acknowledgments

Authors are very grateful to Dr. Gustavo Gasaneo for discussions and his permanent interest to this topics. We are thankful to the Computer Center, Far Eastern Branch of the Russian Academy of Science (Khabarovsk, Russia) and the Computer Center, Université de Lorraine (Metz, France) for generous rendering of computer resources to our disposal.

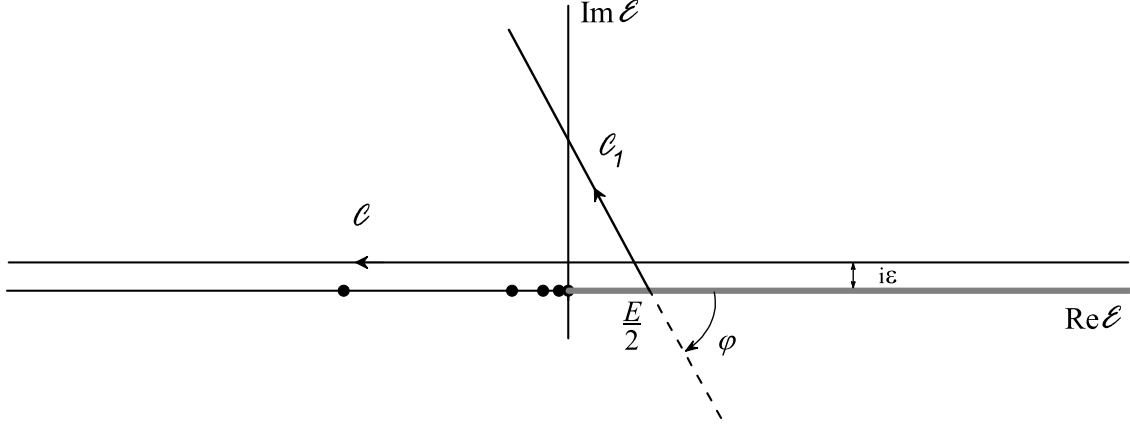


Figure 1:  $\mathcal{C}$  is the straight-line path of integration of the convolution integral (13). The bound-state poles of  $\widehat{G}^{\ell_1(+)}(\sqrt{2\mathcal{E}})$  are depicted as full circles. The grey line is the unitary branch cut. A part of the rotated contour  $\mathcal{C}_1$  (the dashed line) lies in the region of unphysical energies.

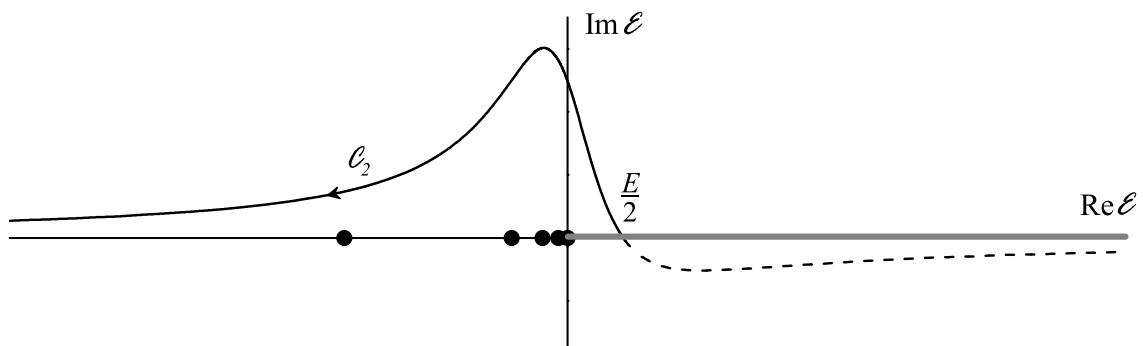


Figure 2: The deformed contour  $\mathcal{C}_2$  asymptotically approaches the real energy axis.

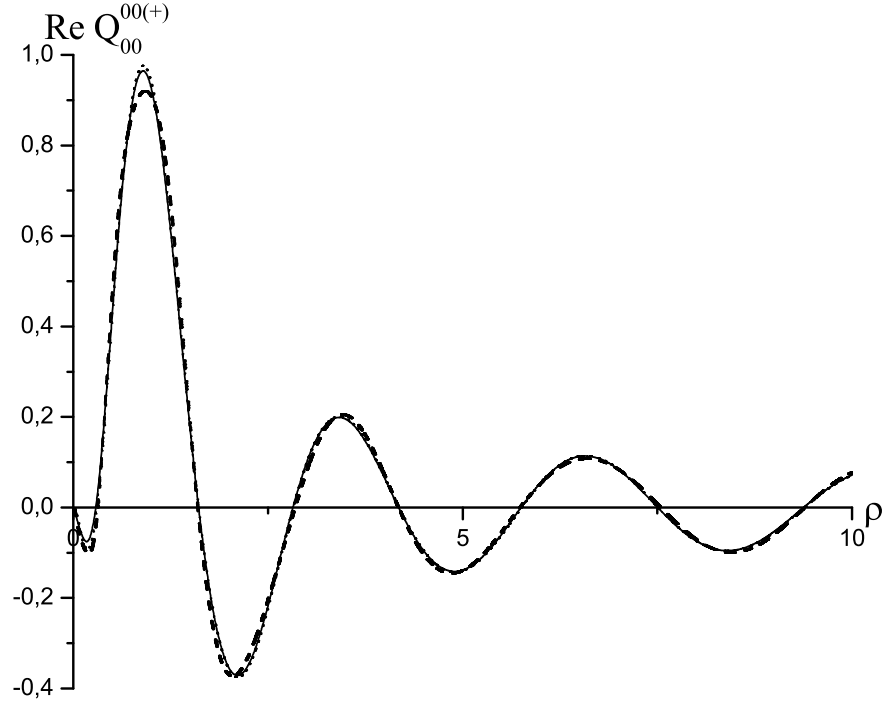


Figure 3: The real part of the  $s$ -wave CQS function  $Q_{00}^{00(+)}$  for  $E = 0.735$  and  $b = 1.6875$  along the diagonal  $r_1 = r_2 = \rho/\sqrt{2}$ , approximated by (16) with the upper limit 25 (dashed line) and obtained by integrating (14) along the contour  $\mathcal{C}_2$  (27) with  $D = 0.85$  (solid line) and  $D = 15$  (dotted line) using the analytic continuation.



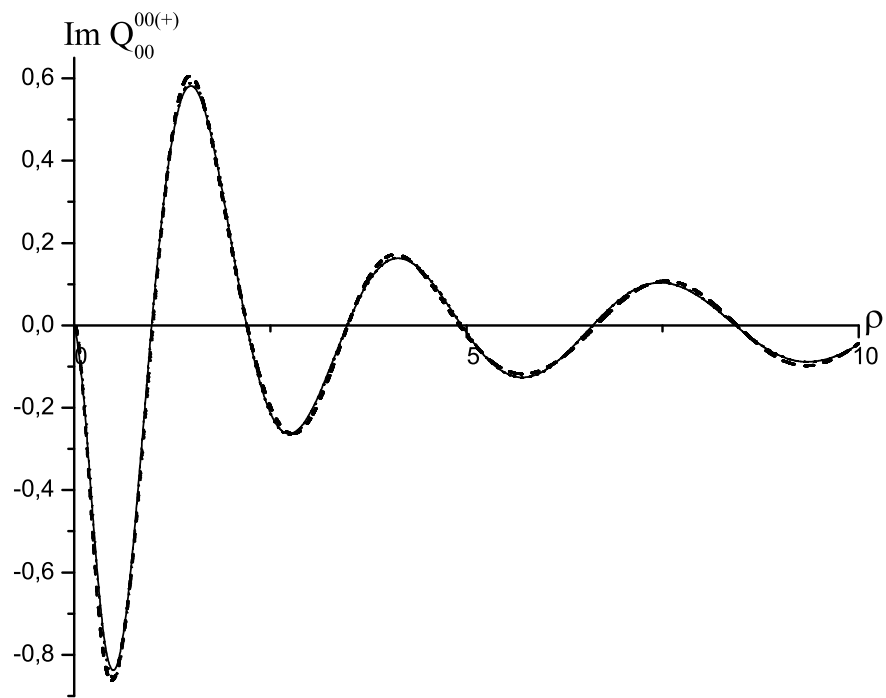


Figure 4: The same as in Fig. 3 but for the imaginary part.

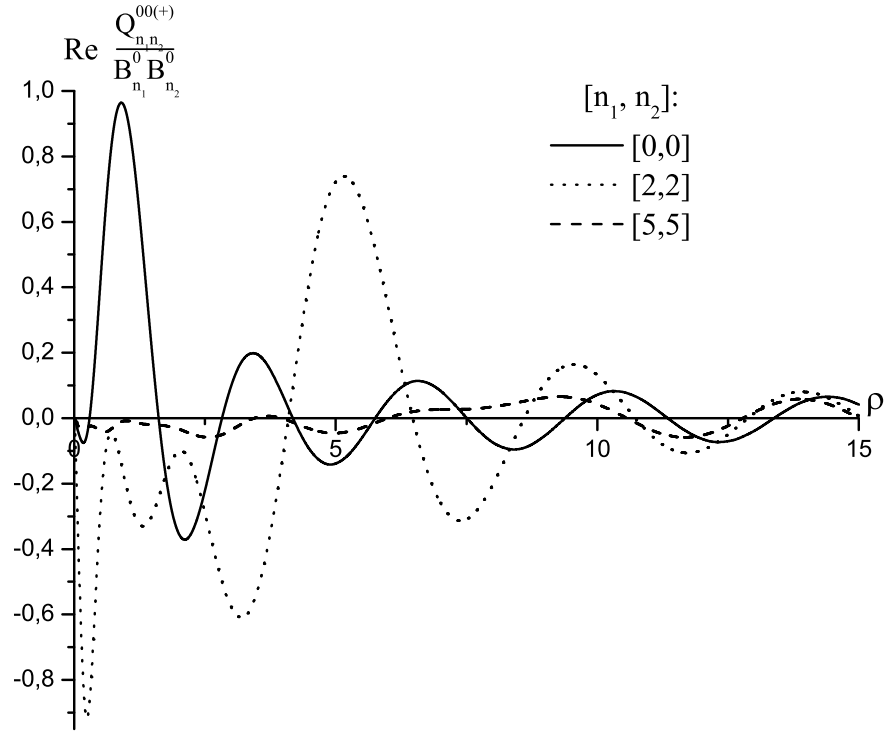


Figure 5: Real parts for the first few  $s$ -wave CQS functions  $\frac{Q_{n_1 n_2}^{00(+)}(E; r_1, r_2)}{B_{n_1}^0(p_1) B_{n_2}^0(p_2)}$  along the  $r_1 = r_2$  diagonal.

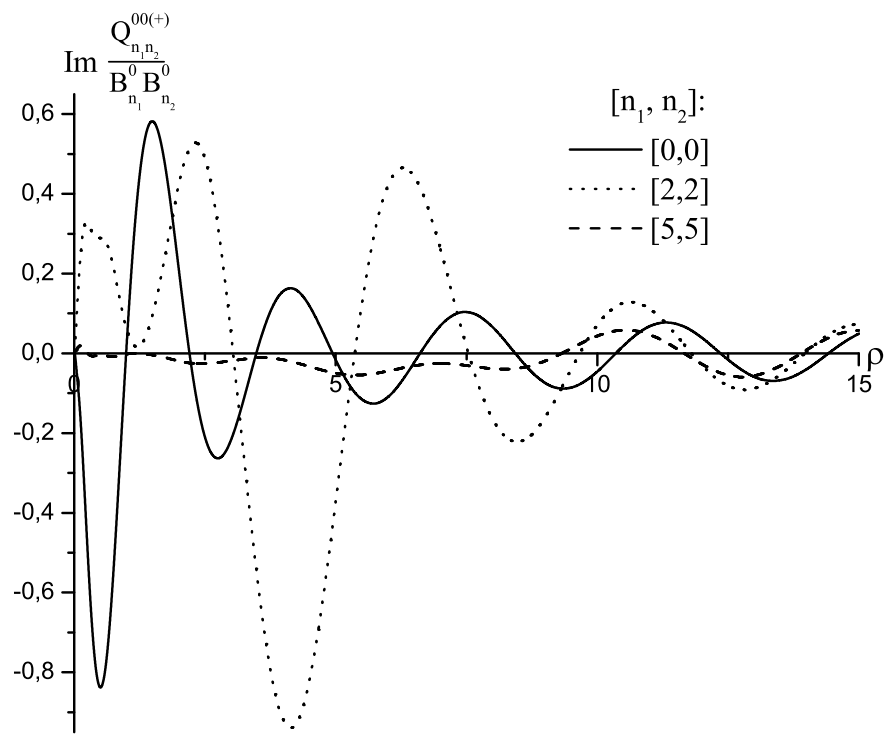


Figure 6: The same as in Fig. 5 but for the imaginary parts.

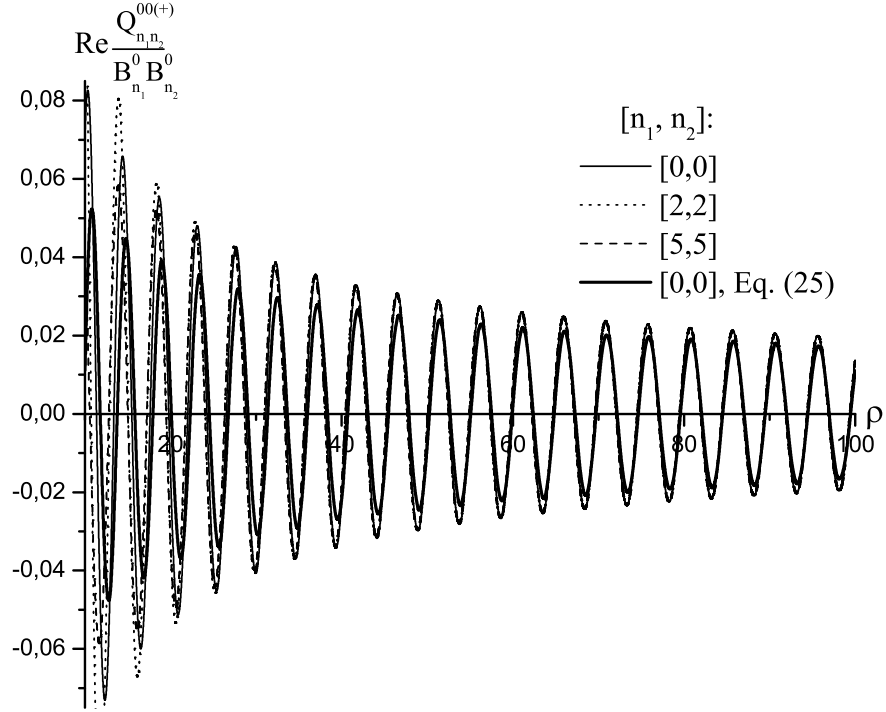


Figure 7: Comparison of the real parts for the first few CQS functions  $\frac{Q_{n_1 n_2}^{00(+)}(E; r_1, r_2)}{B_{n_1}^0(p_1) B_{n_2}^0(p_2)}$  and that of the asymptotic limit (25) for  $Q_{00}^{(00)(+)}$ .

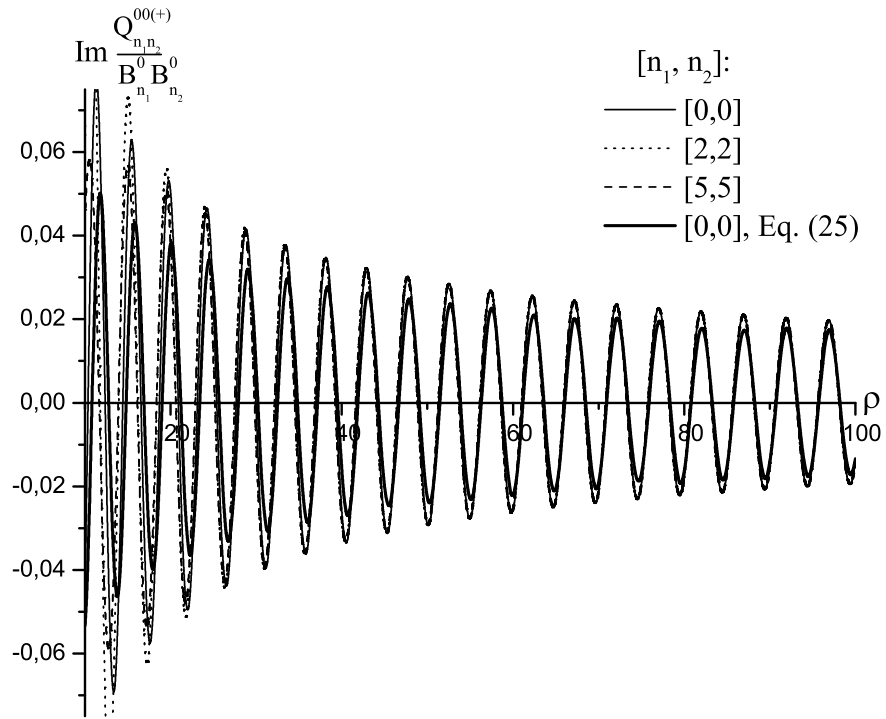


Figure 8: The same as in Fig. 7 but for the imaginary parts.

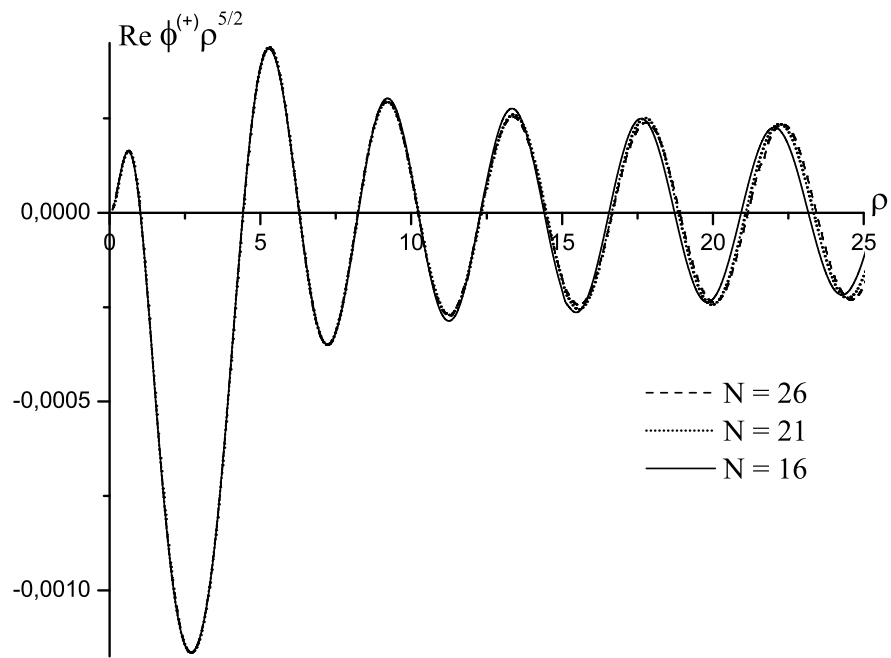


Figure 9: The real components of the solutions  $\phi^{(+)}\rho^{5/2}$  for different basis sizes along the diagonal  $r_1 = r_2$ .

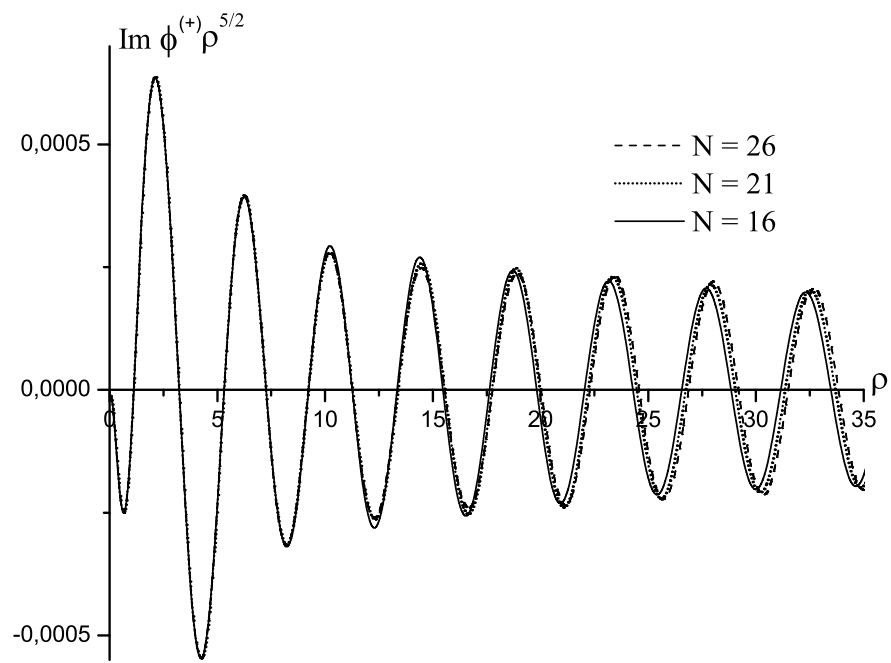


Figure 10: The same as in Fig. 9 but for the imaginary parts.

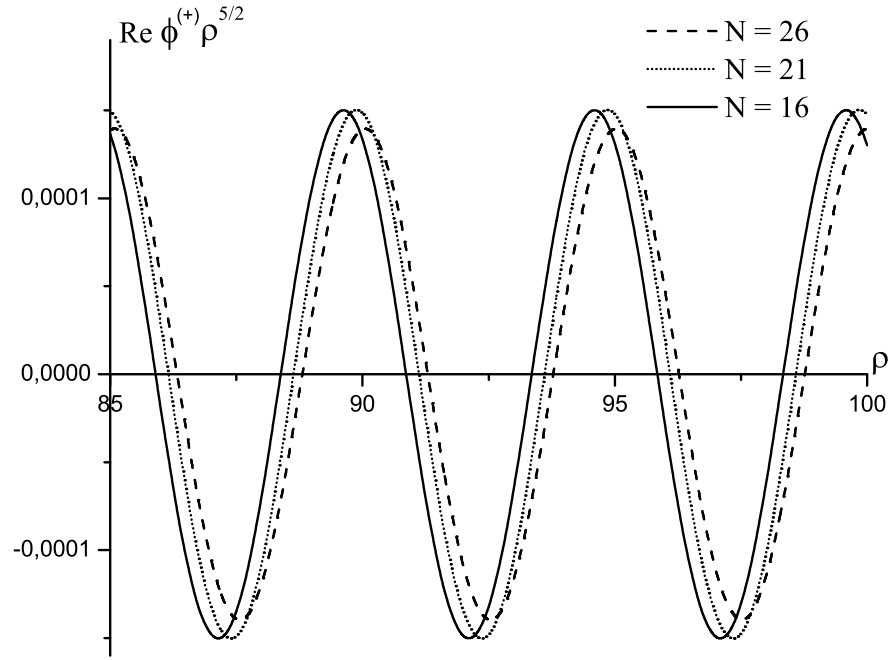


Figure 11: Real parts of the asymptotic form for the solutions  $\phi^{(+)} \rho^{5/2}$  for different basis sizes along the diagonal  $r_1 = r_2$ .



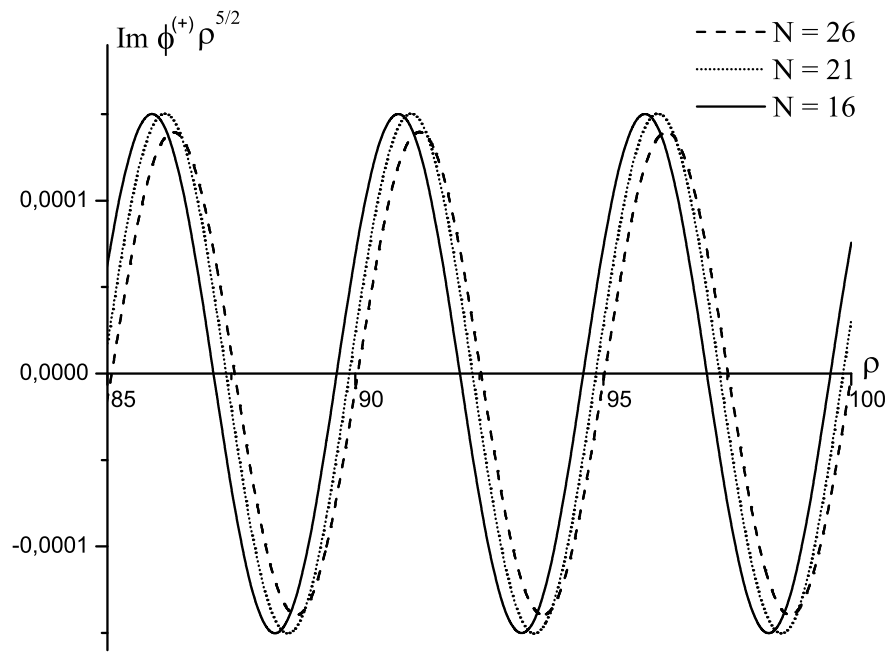


Figure 12: The same as in Fig. 11 but for the imaginary parts.

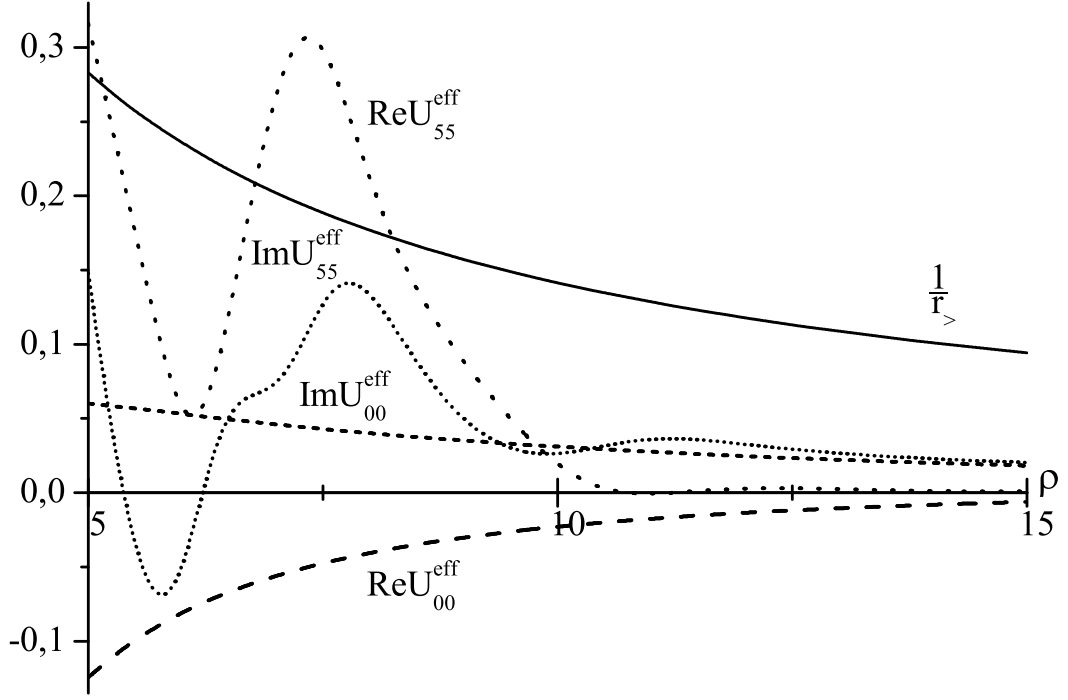


Figure 13: Real and imaginary parts of the ‘effective potentials’  $U_{00}^{\text{eff}}$  and  $U_{55}^{\text{eff}}$  (54).

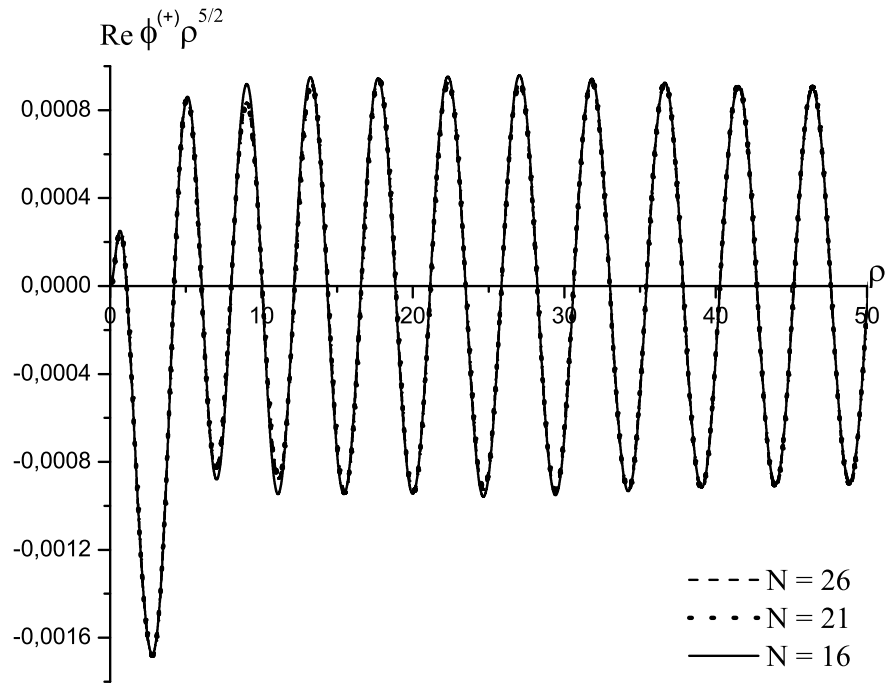


Figure 14: The real components of the solutions  $\tilde{\phi}^{(+)} \rho^{5/2}$  for different basis sizes along the diagonal  $r_1 = r_2$ .

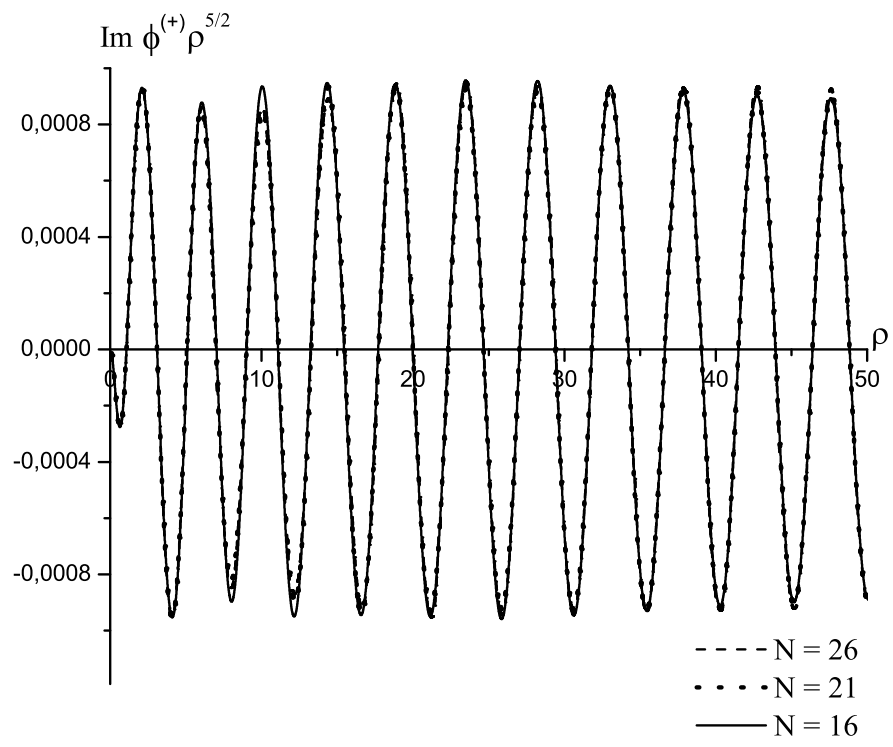


Figure 15: The same as in Fig. 14 but for the imaginary parts.

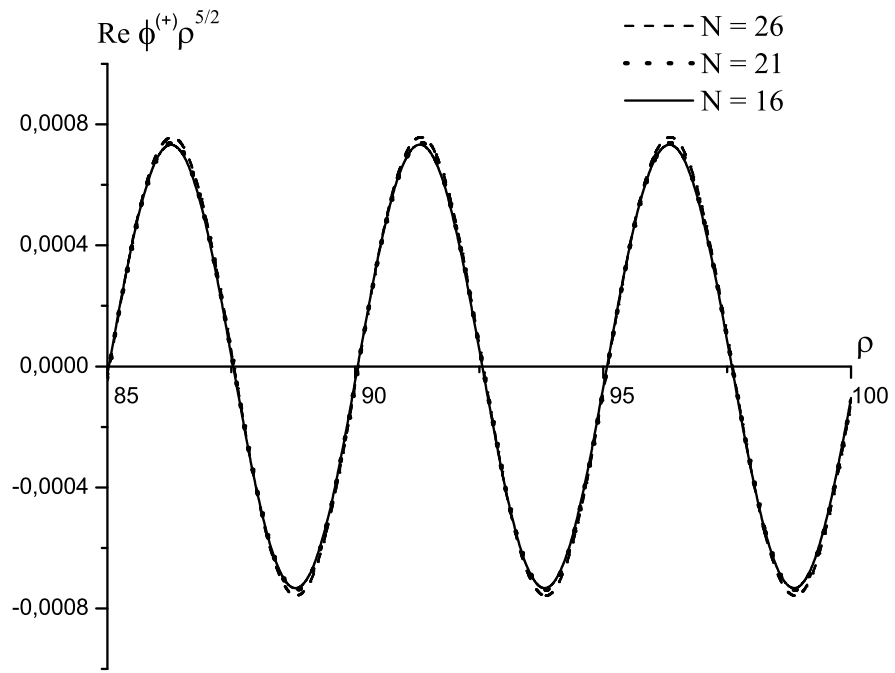


Figure 16: Real parts of the asymptotic form for the solutions  $\tilde{\phi}^{(+)} \rho^{5/2}$  (60) for different basis sizes along the diagonal  $r_1 = r_2$ .

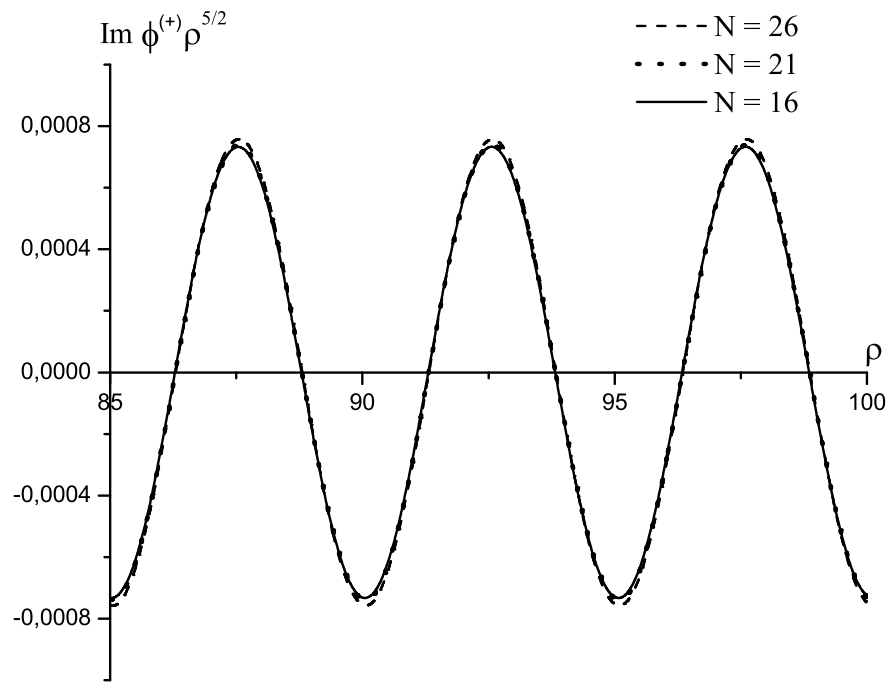


Figure 17: The same as in Fig. 16 but for the imaginary parts.

- 
- [1] I. Bray, D. I. Fursa, A. S. Kadyrov, A. T. Stelbovics, A. Kheifets, and A. M. Mukhamedzhanov, Phys. Rep. **520**, 135 (2012).
  - [2] C. W. McCurdy, M. Baertschy and T. N. Rescigno, J. Phys. B **37**, R137 (2004).
  - [3] M. V. Volkov, N. Elander, E. Yarevsky and S. L. Yakovlev, EPL (Europhysics Letters) **85**, 30001 (2009)
  - [4] N. Elander, M. Volkov, A. Larson, M. Stenrup, J. Z. Mezei, E. Yarevsky, S. Yakovlev, Few-Body Syst. **45**, 197, (2009).
  - [5] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).
  - [6] I. Bray, D. V. Fursa, A. Kheifets, and A. T. Stelbovics, J. Phys. B **35**, R117 (2002).
  - [7] A. S. Kadyrov, A. M. Mukhamedzhanov, A. T. Stelbovics, and I. Bray, Phys. Rev. A **70**, 062703 (2004).
  - [8] Z. Papp, C.-Y. Hu, Z. T. Hlousek, B. Kónya, and S. L. Yakovlev, Phys. Rev. A **63**, 062721 (2001).
  - [9] Z. Papp, J. Darai, C.-Y. Hu, Z. T. Hlousek, B. Kónya, and S. L. Yakovlev, Phys. Rev. A **65**, 032725 (2002).
  - [10] S. A. Zaytsev, V. A. Knyr, Yu. V. Popov, A. Lahmam-Bennani, Phys. Rev. A **75**, 022718 (2007).
  - [11] M. S. Mengoue, M. G. Kwato Njock, B. Piraux, Yu. V. Popov, and S. A. Zaytsev, Phys. Rev. A **83**, 052708 (2011).
  - [12] A. L. Frapiccini, J. M. Randazzo, G. Gasaneo, and F. D. Colavecchia, J. Phys. B **43**, 101001 (2010).
  - [13] G. Gasaneo, L. U. Ancarani, D. M. Mitnik, J. M. Randazzo, A. L. Frapiccini, and F. D. Colavecchia, Adv. Quantum Chem. **67**, 153 (2013).
  - [14] G. Gasaneo, D. M. Mitnik, J. M. Randazzo, L. U. Ancarani, and F. D. Colavecchia, Phys. Rev. A **87**, 042707 (2013).
  - [15] J. A. Del Punta, M. J. Ambrosio, G. Gasaneo, S. A. Zaytsev, and L. U. Ancarani, J. Math. Phys. **55**, 052101 (2014).
  - [16] P. Selles, L. Magelat, A. K. Kazansky, Phys. Rev. A **65**, 032711 (2002).
  - [17] A. Baz, Ya. Zeldovich and A. Perelomov, *Scattering, Reactions, and Decays, in Nonrelativistic*

- Quantum Mechanics* [in Russian] (Nauka, Moscow, 1966); (English. transl., Israel Program for Sci. Translations, Jerusalem, 1969).
- [18] R. Shakehaft, Phys. Rev. A **70**, 042704 (2004).
- [19] E. J. Heller, Phys. Rev. A **12**, 1222 (1975).
- [20] The  $J$ –Matrix Method: Developments and Applications, Ed. by A. D. Alhaidari, E. J. Heller, H. A. Yamani, and M. S. Abdelmonem (Springer Sci., Business Media, 2008).
- [21] S. P. Merkuriev and L. D. Faddeev, *Quantum Scattering Theory for Several Particle Systems* (Kluwer Academic, Dordrecht, 1993).
- [22] M. R. H. Rudge, Rev. Mod. Phys. **40**, 564 (1968).